



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 07:52 AM EST

PDB ID : 6MPD
Title : Citrobacter freundii tyrosine phenol-lyase complexed with 4-hydroxypyridine and aminoacrylate from 3-F-L-tyrosine
Authors : Phillips, R.S.
Deposited on : 2018-10-05
Resolution : 1.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

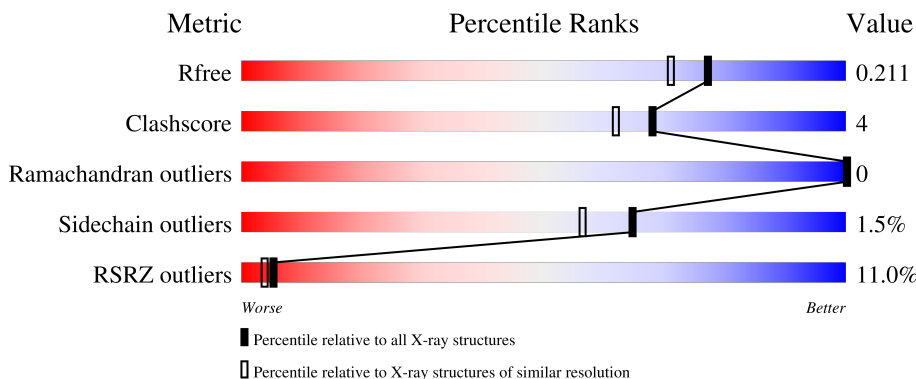
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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)
RSRZ outliers	127900	5850 (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 $\leq 5\%$. 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	456	
2	B	456	

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
7	YOF	B	1602	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8814 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 Tyrosine phenol-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	455	4396	2793	759	814	30	0	95	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	GLU	conflict	UNP P31013

- Molecule 2 is a protein called Tyrosine phenol-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
2	B	455	3714	2349	645	691	1	28	0	13	0

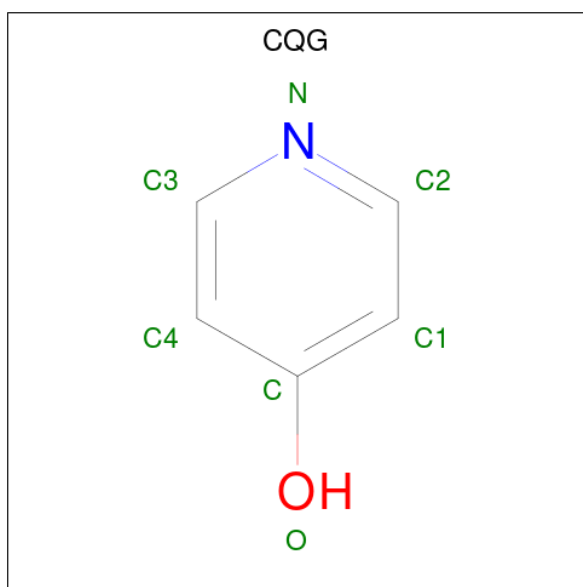
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	205	ALA	GLU	conflict	UNP P31013

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

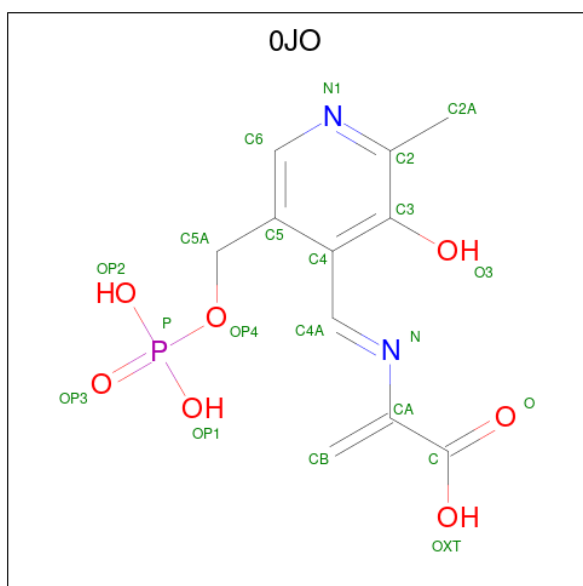
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0

- Molecule 4 is pyridin-4-ol (three-letter code: CQG) (formula: C₅H₅NO).



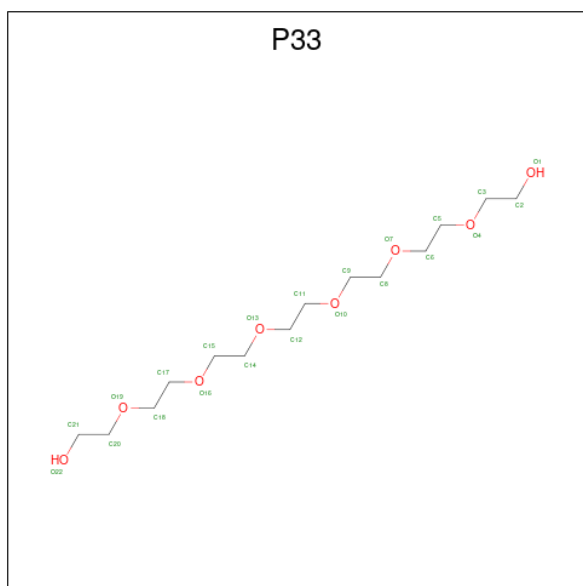
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	5	1	1		
4	A	1	Total	C	N	O	0	0
			7	5	1	1		
4	A	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 5 is 2-[(E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}prop-2-enoic acid (three-letter code: 0JO) (formula: C₁₁H₁₃N₂O₇P).



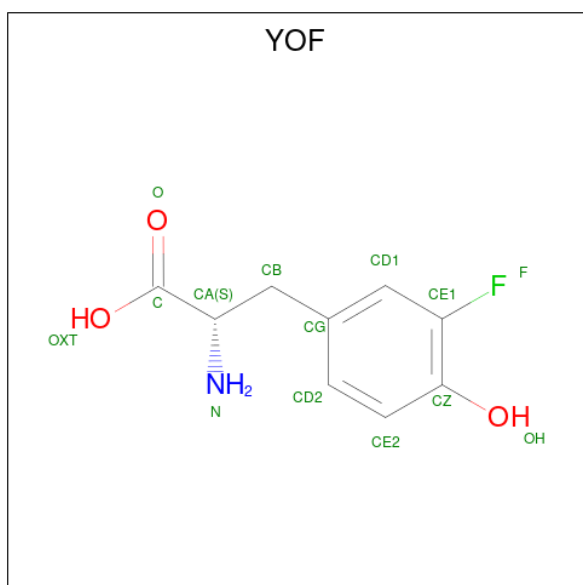
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	21	11	2	7	1	0	0

- Molecule 6 is 3,6,9,12,15,18-HEXAOXAIICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	22	14	8	0	0

- Molecule 7 is 3-FLUOROTYROSINE (three-letter code: YOF) (formula: $C_9H_{10}FNO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
7	B	1	14	9	1	1	3	0	0

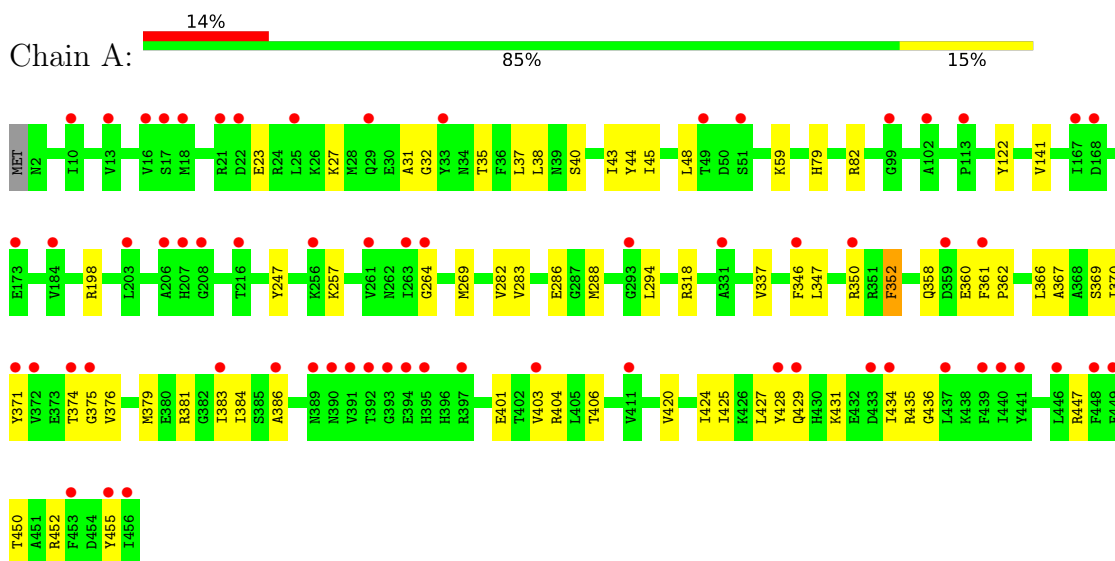
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	302	Total 302	O 302	0	24
8	B	322	Total 322	O 322	0	7

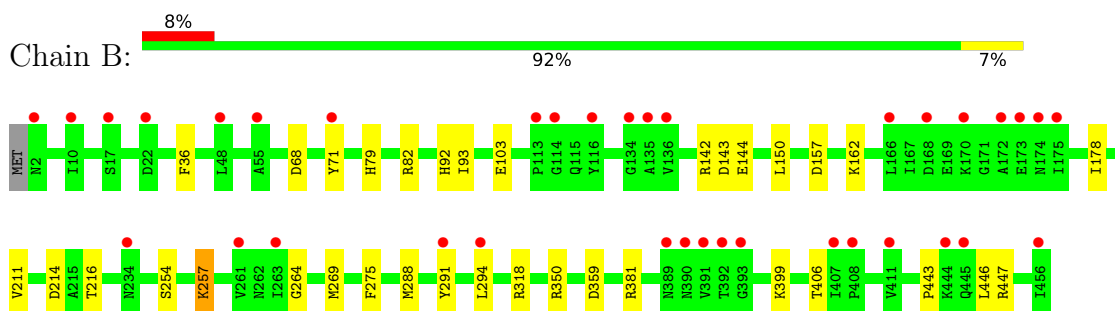
3 Residue-property plots

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: Tyrosine phenol-lyase



- Molecule 2: Tyrosine phenol-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.50Å 133.13Å 143.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.83 – 1.79 38.83 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.83-1.79) 100.0 (38.83-1.79)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.175 , 0.210 0.175 , 0.211	Depositor DCC
R_{free} test set	1985 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.8	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	0.97	EDS
Total number of atoms	8814	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: LLP, YOF, K, P33, CQG, OJO

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	0.37	0/4495	0.54	0/6051
2	B	0.38	0/3784	0.57	1/5092 (0.0%)
All	All	0.37	0/8279	0.55	1/11143 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	68	ASP	CB-CG-OD1	5.30	123.07	118.30

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	4396	0	4337	45	0
2	B	3714	0	3663	17	0
3	A	2	0	0	0	0
4	A	21	0	0	1	0
5	A	21	0	9	3	0
6	B	22	0	30	0	0
7	B	14	0	8	0	0
8	A	302	0	0	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	322	0	0	1	1
All	All	8814	0	8047	61	1

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 4.

All (61) 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:376[B]:VAL:HG21	1:A:420:VAL:HG22	1.71	0.71
1:A:450[B]:THR:O	8:A:1101[B]:HOH:O	2.12	0.66
1:A:352[B]:PHE:O	1:A:431[B]:LYS:HD2	1.97	0.65
1:A:198[A]:ARG:HG2	1:A:247:TYR:CZ	2.38	0.58
1:A:79[A]:HIS:CE1	1:A:82:ARG:HH12	2.22	0.58
1:A:32[B]:GLY:HA3	1:A:452[B]:ARG:HG2	1.87	0.56
1:A:40[B]:SER:HA	1:A:43[B]:ILE:HD12	1.87	0.55
1:A:257:LYS:HZ1	5:A:1004:OJO:C4A	2.20	0.54
1:A:425:ILE:O	1:A:429[B]:GLN:N	2.30	0.54
2:B:264:GLY:HA2	2:B:294:LEU:HD21	1.90	0.54
1:A:347[B]:LEU:HD11	1:A:424:ILE:HD13	1.90	0.54
2:B:216[A]:THR:HG23	2:B:254:SER:HB3	1.89	0.53
2:B:214:ASP:OD1	2:B:216[B]:THR:HG23	2.08	0.53
2:B:350[B]:ARG:NH2	2:B:399:LYS:O	2.41	0.53
2:B:443:PRO:HG2	2:B:447:ARG:HA	1.90	0.53
1:A:358[A]:GLN:NE2	8:A:1110:HOH:O	2.40	0.53
1:A:381:ARG:HG3	1:A:404:ARG:HB2	1.91	0.52
1:A:59:LYS:NZ	8:A:1105:HOH:O	2.33	0.51
1:A:360[B]:GLU:HB3	1:A:436[B]:GLY:HA3	1.94	0.50
1:A:257:LYS:HZ1	5:A:1004:OJO:H4	1.78	0.49
1:A:374[A]:THR:HG22	1:A:376[A]:VAL:HG23	1.94	0.49
2:B:143:ASP:OD1	2:B:162:LYS:NZ	2.36	0.49
1:A:366[A]:LEU:HB3	1:A:403:VAL:HG21	1.95	0.48
1:A:361[A]:PHE:CG	1:A:384:ILE:HD11	2.48	0.48
1:A:427:LEU:O	1:A:431[B]:LYS:HA	2.14	0.48
1:A:257:LYS:NZ	5:A:1004:OJO:C4A	2.76	0.48
1:A:264:GLY:HA2	1:A:294:LEU:HD21	1.95	0.48
2:B:142:ARG:HD2	2:B:157:ASP:HB2	1.96	0.48
1:A:369[B]:SER:HB2	1:A:427:LEU:HD22	1.96	0.47
1:A:350[A]:ARG:HG2	1:A:401:GLU:HB3	1.95	0.47
2:B:350[B]:ARG:NH1	8:B:1712:HOH:O	2.47	0.47
1:A:435[A]:ARG:HB2	1:A:455[A]:TYR:CD1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1003:CQG:N	2:B:71:TYR:OH	2.49	0.46
2:B:103:GLU:OE2	2:B:257:LLP:H6	2.16	0.46
1:A:31[A]:ALA:HB1	1:A:37[A]:LEU:HB2	1.96	0.46
2:B:79[B]:HIS:CD2	2:B:82:ARG:HH22	2.33	0.46
1:A:283:VAL:HG21	2:B:446:LEU:HD21	1.97	0.45
1:A:370[B]:ILE:HG12	1:A:424:ILE:HG12	1.98	0.45
1:A:35[B]:THR:HG21	1:A:367[B]:ALA:HB1	2.00	0.44
1:A:45:ILE:HB	1:A:376[B]:VAL:HG22	1.99	0.44
1:A:362[A]:PRO:HG2	1:A:401:GLU:HG2	1.99	0.44
2:B:144:GLU:HB3	2:B:150:LEU:HD23	1.99	0.44
1:A:371[B]:TYR:O	1:A:375[B]:GLY:HA2	2.17	0.43
1:A:337:VAL:HB	1:A:346[A]:PHE:HB2	2.00	0.43
1:A:383:ILE:O	1:A:447[A]:ARG:NH2	2.51	0.43
2:B:381[B]:ARG:HA	2:B:381[B]:ARG:HD2	1.84	0.43
1:A:337:VAL:HB	1:A:346[B]:PHE:HB2	2.01	0.42
1:A:38[B]:LEU:HD13	1:A:371[B]:TYR:CE1	2.55	0.42
1:A:37[B]:LEU:O	1:A:37[B]:LEU:HD12	2.20	0.42
1:A:31[B]:ALA:HA	1:A:37[B]:LEU:HD11	2.02	0.42
1:A:288:MET:HE2	8:A:1126:HOH:O	2.20	0.42
1:A:23[A]:GLU:O	1:A:27[A]:LYS:HG2	2.20	0.42
1:A:431[B]:LYS:O	1:A:434[B]:ILE:HG22	2.20	0.41
1:A:48[B]:LEU:HD22	1:A:379:MET:HB2	2.01	0.41
1:A:282:VAL:HG22	1:A:286:GLU:HB2	2.03	0.41
1:A:44:TYR:HD2	1:A:374[B]:THR:O	2.03	0.41
1:A:352[B]:PHE:CZ	1:A:428[B]:TYR:HB2	2.56	0.41
2:B:178:ILE:HB	2:B:211:VAL:HG22	2.03	0.41
1:A:122:TYR:OH	1:A:386:ALA:HA	2.20	0.40
2:B:92:HIS:HB3	2:B:275:PHE:CD1	2.56	0.40
2:B:288[B]:MET:HB2	2:B:291:TYR:CD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1262:HOH:O	8:B:2001:HOH:O[2_555]	2.13	0.07

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	547/456 (120%)	539 (98%)	8 (2%)	0	100	100
2	B	465/456 (102%)	456 (98%)	9 (2%)	0	100	100
All	All	1012/912 (111%)	995 (98%)	17 (2%)	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	463/378 (122%)	457 (99%)	6 (1%)	69	62
2	B	389/377 (103%)	383 (98%)	6 (2%)	65	56
All	All	852/755 (113%)	840 (99%)	12 (1%)	65	59

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	VAL
1	A	269	MET
1	A	318	ARG
1	A	352[A]	PHE
1	A	352[B]	PHE
1	A	406	THR
2	B	36	PHE
2	B	93	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	269	MET
2	B	318	ARG
2	B	359	ASP
2	B	406	THR

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](#)

1 non-standard protein/DNA/RNA residue is 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	LLP	B	257	2,7	23,24,25	2.63	6 (26%)	25,32,34	1.33	3 (12%)

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	LLP	B	257	2,7	-	7/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	257	LLP	C4-C4'	8.55	1.62	1.46
2	B	257	LLP	C4'-NZ	5.54	1.45	1.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	257	LLP	C2'-C2	3.55	1.56	1.50
2	B	257	LLP	C4-C5	-2.97	1.38	1.42
2	B	257	LLP	C6-N1	2.51	1.39	1.34
2	B	257	LLP	C3-C2	2.03	1.42	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	257	LLP	C4-C4'-NZ	-2.85	111.22	124.31
2	B	257	LLP	C5'-C5-C6	-2.79	114.79	119.37
2	B	257	LLP	C5-C6-N1	-2.36	119.89	123.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	257	LLP	C3-C4-C4'-NZ
2	B	257	LLP	C4-C4'-NZ-CE
2	B	257	LLP	O-C-CA-CB
2	B	257	LLP	CA-CB-CG-CD
2	B	257	LLP	CE-CD-CG-CB
2	B	257	LLP	CD-CE-NZ-C4'
2	B	257	LLP	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	257	LLP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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
7	YOF	B	1602	2	13,14,14	2.01	3 (23%)	16,19,19	1.81	5 (31%)
6	P33	B	1601	-	21,21,21	0.54	0	20,20,20	0.22	0
4	CQG	A	1002	-	7,7,7	3.88	3 (42%)	8,8,8	0.90	0
4	CQG	A	1006	-	7,7,7	3.88	5 (71%)	8,8,8	0.96	0
4	CQG	A	1003	-	7,7,7	3.94	5 (71%)	8,8,8	0.97	1 (12%)
5	0JO	A	1004	-	20,21,21	2.33	9 (45%)	23,30,30	1.24	3 (13%)

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
7	YOF	B	1602	2	-	3/8/8/8	0/1/1/1
6	P33	B	1601	-	-	11/19/19/19	-
4	CQG	A	1002	-	-	-	0/1/1/1
4	CQG	A	1006	-	-	-	0/1/1/1
4	CQG	A	1003	-	-	-	0/1/1/1
5	0JO	A	1004	-	-	0/10/15/15	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1006	CQG	O-C	-6.17	1.22	1.37
4	A	1002	CQG	O-C	-5.88	1.23	1.37
4	A	1003	CQG	O-C	-5.77	1.23	1.37
4	A	1003	CQG	C4-C	5.63	1.49	1.38
4	A	1003	CQG	C1-C	5.61	1.49	1.38
4	A	1002	CQG	C4-C	5.50	1.49	1.38
4	A	1002	CQG	C1-C	5.45	1.49	1.38
4	A	1006	CQG	C1-C	5.33	1.49	1.38
5	A	1004	0JO	C4-C5	-5.11	1.35	1.42
4	A	1006	CQG	C4-C	5.02	1.48	1.38
7	B	1602	YOF	O-C	5.01	1.37	1.22
7	B	1602	YOF	CZ-CE1	4.05	1.42	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1004	OJO	C2A-C2	-3.78	1.44	1.50
5	A	1004	OJO	OP4-C5A	-3.63	1.31	1.45
5	A	1004	OJO	O3-C3	-3.61	1.28	1.37
5	A	1004	OJO	C3-C2	-3.36	1.37	1.40
4	A	1006	CQG	C4-C3	-2.55	1.33	1.38
5	A	1004	OJO	C4-C3	-2.38	1.37	1.40
5	A	1004	OJO	OXT-C	-2.31	1.23	1.30
4	A	1006	CQG	C1-C2	-2.26	1.34	1.38
5	A	1004	OJO	P-OP2	-2.21	1.46	1.54
4	A	1003	CQG	C4-C3	-2.11	1.34	1.38
5	A	1004	OJO	P-OP1	-2.11	1.46	1.54
7	B	1602	YOF	CD1-CE1	2.05	1.41	1.37
4	A	1003	CQG	C1-C2	-2.03	1.34	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1602	YOF	OXT-C-CA	4.36	128.24	113.38
7	B	1602	YOF	CG-CB-CA	3.20	120.78	114.13
5	A	1004	OJO	C4-C4A-N	-3.02	115.85	123.19
7	B	1602	YOF	OXT-C-O	-2.53	118.35	124.09
7	B	1602	YOF	O-C-CA	-2.48	113.40	122.14
7	B	1602	YOF	CG-CD1-CE1	2.18	120.78	119.37
4	A	1003	CQG	C2-N-C3	2.15	121.91	116.85
5	A	1004	OJO	OP1-P-OP4	-2.13	101.06	106.73
5	A	1004	OJO	OP2-P-OP1	2.03	115.39	107.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1601	P33	O10-C11-C12-O13
6	B	1601	P33	O4-C5-C6-O7
6	B	1601	P33	C11-C12-O13-C14
6	B	1601	P33	O7-C8-C9-O10
6	B	1601	P33	O13-C14-C15-O16
6	B	1601	P33	C17-C18-O19-C20
7	B	1602	YOF	O-C-CA-CB
7	B	1602	YOF	OXT-C-CA-CB
6	B	1601	P33	C15-C14-O13-C12
6	B	1601	P33	O19-C20-C21-O22
6	B	1601	P33	C18-C17-O16-C15

Continued on next page...

Continued from previous page...

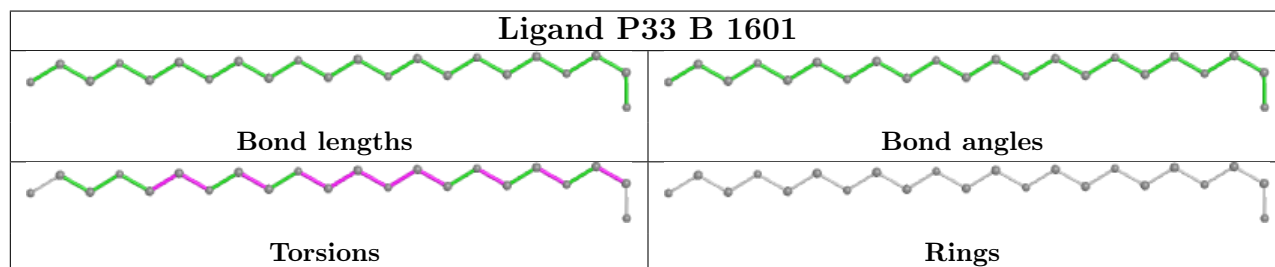
Mol	Chain	Res	Type	Atoms
6	B	1601	P33	C5-C6-O7-C8
6	B	1601	P33	C12-C11-O10-C9
7	B	1602	YOF	OXT-C-CA-N

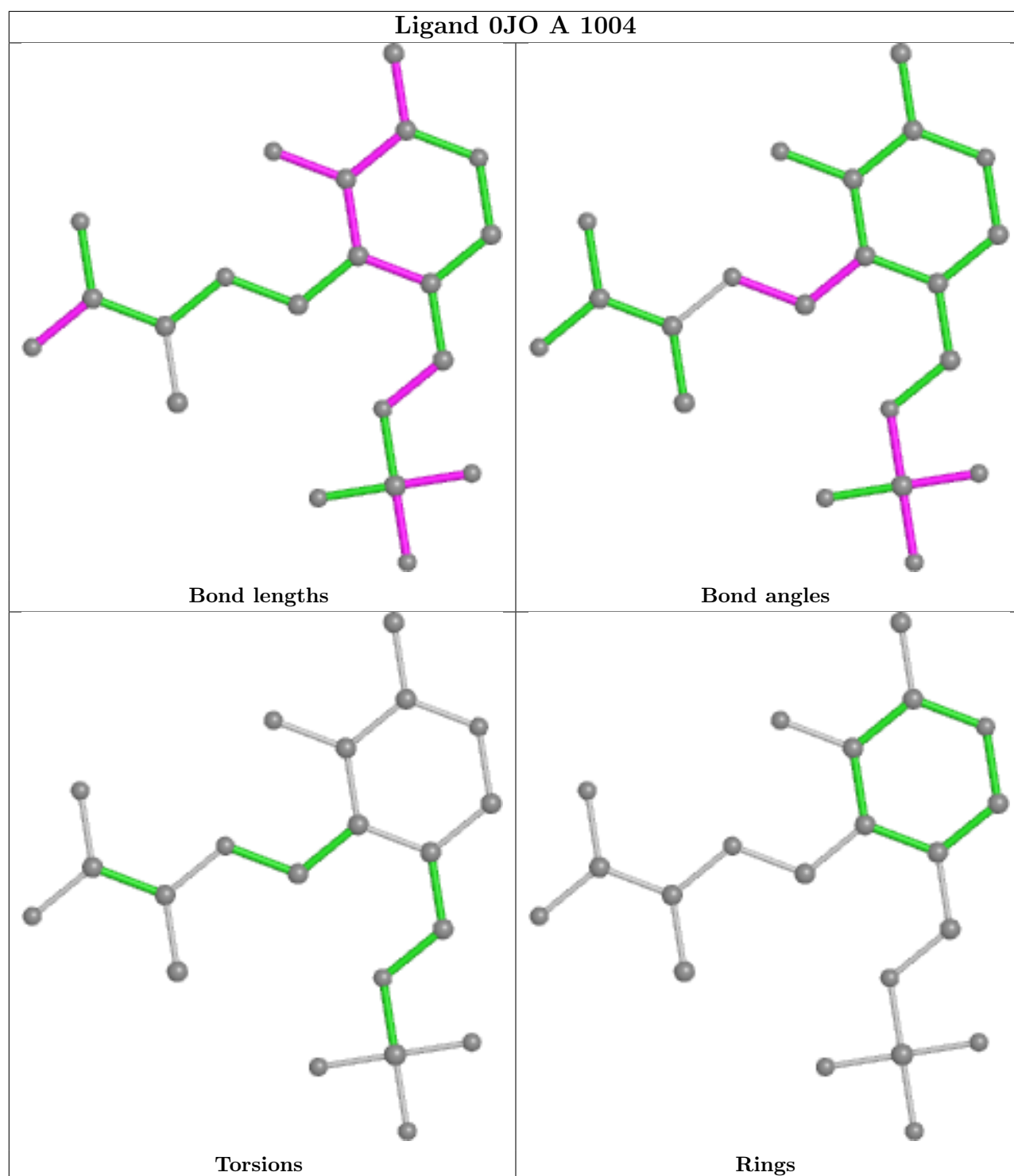
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	CQG	1	0
5	A	1004	OJO	3	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	455/456 (99%)	0.77	64 (14%) 2 1	27, 47, 77, 141	0
2	B	454/456 (99%)	0.28	36 (7%) 12 9	30, 45, 68, 108	0
All	All	909/912 (99%)	0.53	100 (11%) 5 4	27, 45, 73, 141	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	VAL	11.7
2	B	391	VAL	9.3
1	A	456[A]	ILE	7.4
2	B	390	ASN	6.8
1	A	446[A]	LEU	5.8
1	A	392	THR	5.7
1	A	449[A]	PHE	4.8
1	A	25[A]	LEU	4.6
2	B	456	ILE	4.5
1	A	389	ASN	4.4
1	A	22[A]	ASP	4.4
2	B	173	GLU	4.3
2	B	116	TYR	4.3
1	A	113	PRO	4.3
1	A	371[A]	TYR	4.3
2	B	2	ASN	4.3
1	A	168	ASP	4.2
1	A	393	GLY	4.0
1	A	167	ILE	4.0
1	A	184	VAL	3.9
1	A	437[A]	LEU	3.9
1	A	361[A]	PHE	3.8
1	A	440[A]	ILE	3.8
1	A	263	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	383	ILE	3.6
2	B	172	ALA	3.6
1	A	394	GLU	3.6
1	A	390	ASN	3.5
2	B	411	VAL	3.5
1	A	428[A]	TYR	3.5
1	A	411	VAL	3.3
1	A	203	LEU	3.3
1	A	375[A]	GLY	3.3
2	B	166	LEU	3.2
1	A	397	ARG	3.2
1	A	173	GLU	3.2
2	B	17[A]	SER	3.1
2	B	392	THR	3.1
2	B	407	ILE	3.0
2	B	174	ASN	3.0
1	A	372[A]	VAL	3.0
1	A	18[A]	MET	3.0
1	A	33[A]	TYR	2.9
2	B	134	GLY	2.9
1	A	206	ALA	2.8
2	B	393	GLY	2.8
1	A	455[A]	TYR	2.8
2	B	261	VAL	2.8
1	A	29[A]	GLN	2.8
2	B	263	ILE	2.8
1	A	434[A]	ILE	2.7
2	B	113	PRO	2.7
2	B	234	ASN	2.7
1	A	374[A]	THR	2.7
1	A	448[A]	PHE	2.7
2	B	114	GLY	2.6
2	B	175	ILE	2.6
1	A	386	ALA	2.6
1	A	453[A]	PHE	2.6
1	A	261	VAL	2.5
2	B	55	ALA	2.4
2	B	294	LEU	2.4
2	B	168	ASP	2.4
2	B	10	ILE	2.4
2	B	22[A]	ASP	2.4
2	B	48	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	408	PRO	2.3
1	A	99	GLY	2.3
1	A	293	GLY	2.3
2	B	170	LYS	2.3
1	A	256	LYS	2.3
1	A	441[A]	TYR	2.3
1	A	429[A]	GLN	2.3
1	A	439[A]	PHE	2.3
2	B	71	TYR	2.3
1	A	264	GLY	2.3
2	B	136	VAL	2.2
2	B	445	GLN	2.2
1	A	331	ALA	2.2
1	A	208	GLY	2.2
1	A	216	THR	2.2
1	A	433[A]	ASP	2.2
1	A	51	SER	2.2
2	B	444	LYS	2.2
1	A	359[A]	ASP	2.1
1	A	13	VAL	2.1
1	A	16[A]	VAL	2.1
2	B	135	ALA	2.1
1	A	10	ILE	2.1
1	A	49	THR	2.1
1	A	350[A]	ARG	2.1
2	B	291	TYR	2.1
1	A	102	ALA	2.1
1	A	17[A]	SER	2.1
1	A	395	HIS	2.0
2	B	389	ASN	2.0
1	A	21[A]	ARG	2.0
1	A	207	HIS	2.0
1	A	403	VAL	2.0
1	A	346[A]	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
2	LLP	B	257	24/25	0.98	0.14	31,37,58,64	0

6.3 Carbohydrates [i](#)

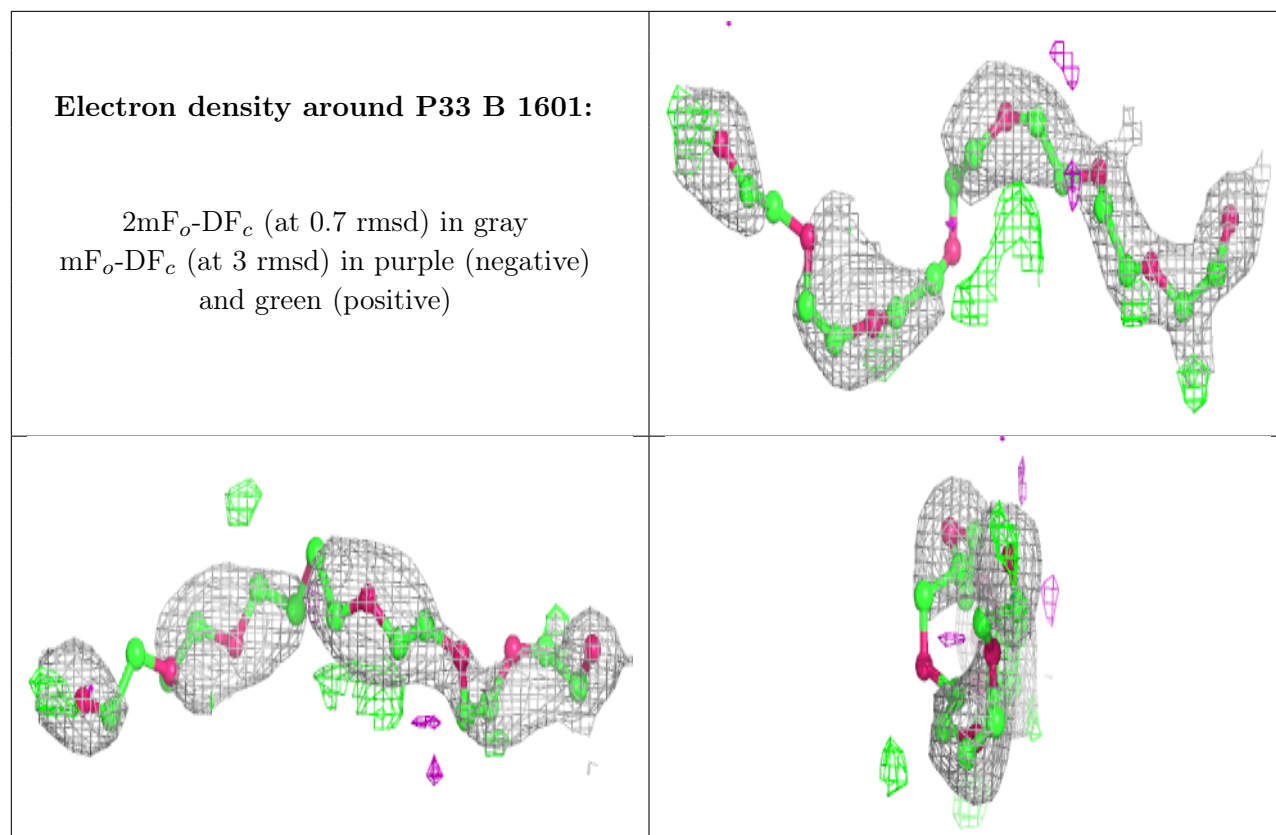
There are no monosaccharides in this entry.

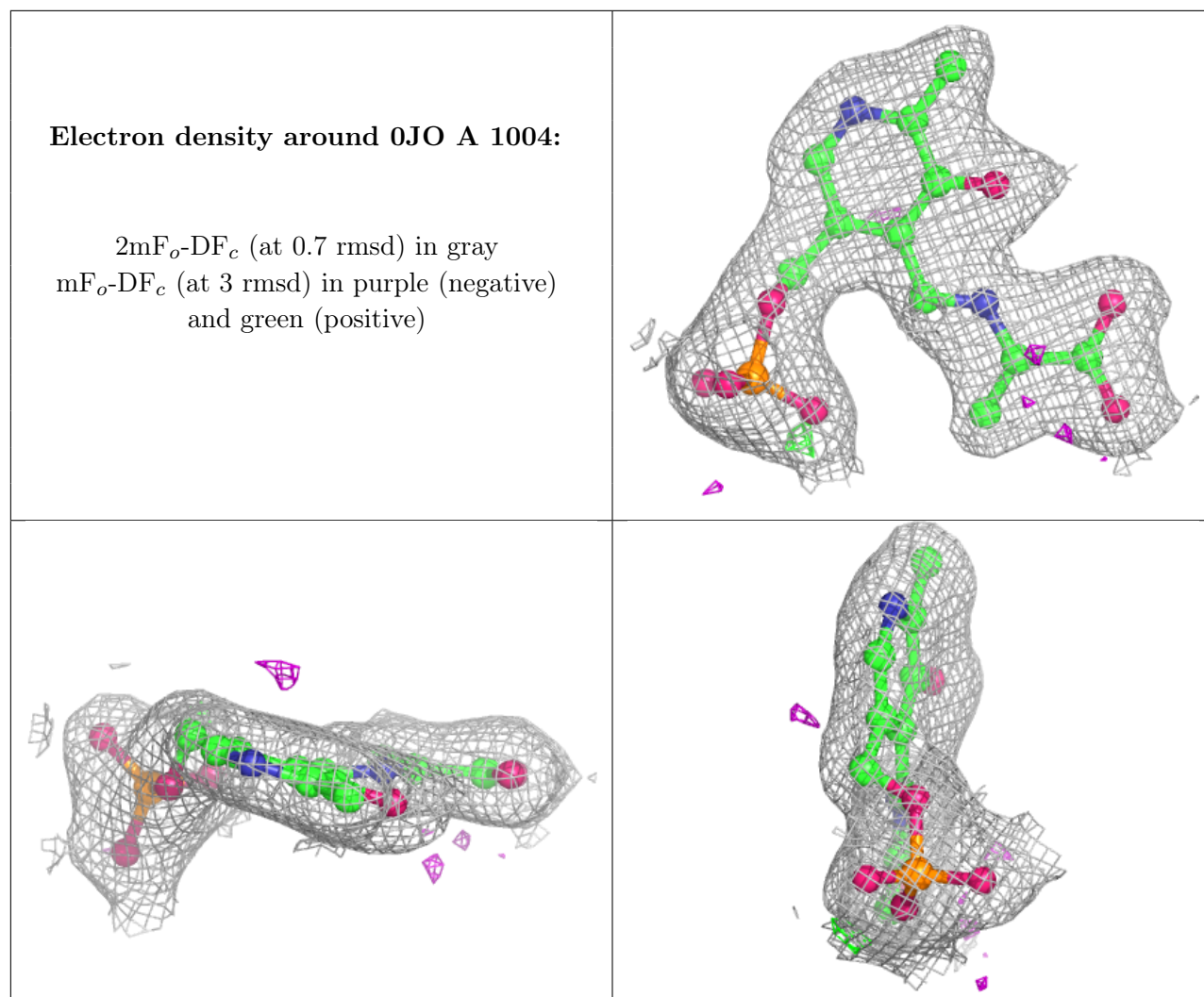
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
6	P33	B	1601	22/22	0.54	0.26	71,91,95,98	0
7	YOF	B	1602	14/14	0.75	0.47	45,54,58,59	14
4	CQG	A	1002	7/7	0.84	0.18	72,74,77,77	0
4	CQG	A	1006	7/7	0.84	0.29	74,77,78,80	7
4	CQG	A	1003	7/7	0.88	0.22	49,51,53,55	7
5	OJO	A	1004	21/21	0.97	0.15	33,38,44,48	0
3	K	A	1005	1/1	0.98	0.09	35,35,35,35	0
3	K	A	1001	1/1	1.00	0.11	36,36,36,36	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.